

A NEW MODEL FOR PREDICTING THE FOULING DEPOSIT WEIGHT OF COAL

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INTRODUCTION

One of the major problems associated with coal combustion is the buildup of sintered ash deposits in the convective passes of boilers. These deposits, referred to as fouling deposits, can drastically reduce heat transfer, cause erosion by channelizing gas flow, and contribute to the corrosion of exposed metal surfaces. Downtime for cleaning fouled commercial boilers can be a multi-million-dollar expense (1).

Utility boilers generally are designed to burn coal that falls within a specific fouling behavior range. Therefore, to minimize the deleterious effects of boiler fouling and to maximize boiler efficiency, it is necessary to anticipate or assess the fouling characteristics of a coal prior to combustion.

This paper introduces a new method for predicting fouling deposit weights by using commonly available coal quality data.

We have developed a modified concept of the coal quality characteristics that influence fouling. This concept evolved from a review of the literature and from the statistical analysis of results from 44 combustion tests.

COAL-FOULING-ASSESSMENT INDICES

Several fouling indices based on ash chemistry have been proposed (2). Most are applicable to coal with eastern, or bituminous, ash.* These indices have met with mixed success. Wall et al. (3) state that "there may be very severe limitations to the applicability of 'fouling indices' based on elemental analysis or even on fusion observations...." Moreover, Wall et al. (3, p. 8) note that at a conference on combustion "a number of speakers stated that fouling indices they had used appeared applicable only to coal from a particular field."

*For technological purposes, coals in which the sum of the calcium oxide and magnesium oxide content is greater than the ferric oxide content are characterized as having "eastern" or "bituminous" ash. The relationship is reversed for coals characterized as having "western" or "lignitic" ash.

One reason for the lack of success in applying the fouling indices is that fouling deposits are formed from a complex series of physical and chemical interactions involving several chemical constituents in the coal. The fouling indices, however, focus on only a few of these constituents and put major emphasis on the sodium content.

METHODS

The data used in this study were supplied by the University of North Dakota Energy Research Center (UNDERC) in Grand Forks, North Dakota. The UNDERC supplied the results from over 200 combustion tests conducted in a pilot-scale test combustor. In addition to the combustion test results, the UNDERC also provided complete characterization of the coal samples tested, and the combustion conditions maintained during the course of each test. Coal characterization included proximate, ultimate, and ash composition information. Table 1 shows the coal composition values and combustion test results used as variables in our study.

We selected a set of 44 samples from the raw data provided by UNDERC. This data set served as the basis for developing the model for fouling deposit prediction. The development data set 1) is representative of the UNDERC data set containing data on lignites and subbituminous coals predominantly from the Northern Great Plains Coal Province, 2) contains at least one observation from each mine or locality represented in the UNDERC file, 3) has no sample duplication, 4) is taken from samples that exhibit a wide range of compositions and fouling behaviors, and 5) had similar combustion test conditions.

Our goal was to use the development data set to model fouling deposit weight in grams per million Btu by using coal quality parameters as independent variables. Coal feed rates and total coal burned in a test could vary from test to test, depending upon the calorific value of the coal. Therefore, conversion of deposit weights to a weight per million Btu basis puts the fouling tendency on a unit energy input basis, a basis frequently used by boiler operators for other purposes such as evaluating sulfur emissions.

The first step in data analysis was to determine if the natural frequency distributions of the variables in the development data set approximate a normal frequency distribution. In all statistical analyses, we assumed the variables to be approximately normally distributed. Therefore, the variables that, in their original form, were not normally distributed were mathematically transformed to yield frequency distributions that approximated normal distribution. The transform functions (Table 1) for each variable were used in all subsequent analysis.

The second step in our study was to conduct bivariate analyses, i.e., calculation and interpretation of correlation coefficients (r -squared values). This analysis determined which variables most closely correlate with fouling deposit weight.

The third and principal step in our analysis was to employ multiple regression analysis to develop a model. We used the STEPWISE, RSQUARE, and REG procedures in SAS (4) to develop and evaluate possible models. All of these

procedures are linear least-squares methods for establishing empirical relationships between one or more independent variables and some response variable. In our case, the independent variables, or regressor variables, are transformed coal-quality parameters. The response variable is the log function of the fouling deposit weight in grams of deposit per million Btu fired.

Models were evaluated on the basis of the improvement in r-squared values, the decrease in the residual sum of squares, the significance of parameter estimates for each variable, and the linkage between fouling behavior and each variable being considered. Statistical significance alone was not enough to include a variable in the model. The final model selected was one that maximized the fit of the predicted values to the actual fouling deposit weight values; thus, maximizing the r-squared value and minimizing the sum of squared residuals.

Finally, we tested the model. For this purpose, we selected a second set of observations from the raw UNDERC data set. This set had the same characteristics as the development data set but contained only 15 samples and had no observations in common with the original data set. We tested the model by calculating a predicted fouling deposit weight using the model and then by comparing the calculated deposit weight with the actual deposit weight.

RESULTS

Bivariate Analysis

In the process of calculating the correlation coefficients for the variables in the development data set we discovered that several coal compositional parameters have significant correlation with fouling deposit weight (Table 2). The amount of ash, total sulfur, titania (TiO_2), potash (K_2O), silicon (Si), sodium (Na), aluminum (Al), and the alkali ratio are significantly related to fouling deposit weight. However, even though the correlations are significant at the 1-percent confidence level, the correlation coefficients are not very high indicating that no one variable is principally responsible for variation in fouling deposit weight. The relationship between fouling and coal composition is too complex to explain with just one variable. This relation is illustrated by means of a few scatter plot diagrams, one showing sodium versus deposit weight (Fig. 1) and the other showing ash yield versus deposit weight (Fig. 2).

Sodium, at present, is the most widely used predictor of fouling tendency; yet, Figure 1 demonstrates that low sodium oxide content in a coal does not guarantee low fouling or that high sodium oxide content equates with severe fouling. Obviously, fouling behavior is dependent upon something other than, or in addition to, the sodium oxide content of coal.

Figure 2 shows the dry ash yield of a coal plotted against the coal's fouling deposit weight. The relationship here is more linear than the one observed for Na_2O , therefore, as ash yield increases so too should fouling deposit weight. This may be thought of as the boiler tubes being exposed to more potential fouling material per unit energy generated. However, the

significant scatter in the relationship of ash yield and deposit weight would preclude the use of only ash as a predictor.

Both sodium (5) and ash yield have been shown to enhance fouling behavior (6). If we plot sodium, ash, and deposit weight on a three-dimensional diagram (Figure 3) we can see the relative influence of the two variables on deposit weight.

Figure 3 indicates that low sodium, low ash coals are low fouling coals. High fouling coals are having with moderate to low amounts of sodium but high ash yields. Deposit weights are more variable when ash yields are low to moderate and sodium values are moderate to high.

The use of ash and sodium together as predictors of fouling may be more reliable than the use of sodium alone, however, we had reliable predictions only in end member situations (low sodium, very high ash). One or two coal composition variables cannot adequately explain or predict fouling behavior. Consequently, we used multiple regression analysis to develop a model to explain the variation of fouling deposit weight values in the development data set.

THE REGRESSION MODEL.

The regression model we found that best fits the fouling deposit weights in the development data set is given in equation 1. The variables incorporated into the model and their basis are listed in Table 3. The model calculates the logarithm of the fouling deposit weight in terms of grams of deposit per million Btu fired and it incorporates TiO_2 , total sulfur, ash yield, Ca/S, and a factor called the alkali ratio. This latter term is calculated by using calcium, magnesium, sodium, and potassium oxide values and the ash yield. The fouling prediction equation is:

$$\log_{10}(FDW) = 1.21 + 0.45 (\log_{10}Ti) + 1.46 (\log_{10}S) + 0.38 (\log_{10}ASH) + 1.14 (\log_{10}Ca/S) + 0.63 (\log_{10}ALK) \quad (1)$$

Where: **FDW** = Fouling Deposit Weight (grams/million Btu)

Ti = Titanium Dioxide % (sulfate-free ash)

S = Sulfur % (dry coal)

ASH = Ash Yield % (dry coal)

Ca/S = Calcium/Sulfur (both % wt. of dry coal)

Ash % (dry * $(Na_2O + .659K_2O)$)

****ALK** = $\frac{\text{Ash \% (dry * (Na}_2\text{O + .659K}_2\text{O))}}{\text{CaO + MgO}}$ (alkali ratio)

**** Na_2O , K_2O , CaO , and MgO are all on a % of sulfate-free ash basis.**

To use the model, the coal quality information required is: ash yield (percent dry coal), sulfur (percent dry coal), and titanium, sodium, calcium, potassium, and magnesium oxides (percent sulfate-free ash). The calcium-sulfur ratio and the alkali ratio are then calculated. Then the logarithm of each parameter in Table 3 is calculated and inserted in equation 1. The result of the calculation is the base 10 logarithm of the fouling deposit weight. This can then be converted directly to grams deposit per million Btu, the predicted fouling deposit weight.

In Figure 4, predicted and observed deposit weight values are plotted. The proximity of the points to the parity line indicates that the model and actual data are in good agreement. Also, the r-squared value, 0.84, is high and significant and indicates that a significant amount of the variability in actual fouling deposit weight is explained or accounted for by the model. The sum of the squared residuals is 1.35. This value is low relative to those obtained for other potential models that we tested. In addition, all of the variables included in the model, except the calcium-sulfur ratio, correlate with fouling deposit weight.

TESTING THE MODEL

Our test of the regression model using the smaller test data set shows that the model works well. The actual versus predicted fouling deposit weights for the test samples are plotted in Figure 5. As with the development data set, points are clustered along the parity line. However, for the test data, the r-squared value is lower than that calculated for the development data because the range in values in the test data set is more limited and there are fewer observations.

We recognize that the model is subject to error. The plots are on a logarithmic scale thus small deviations from the parity line could result in errors of several 10's of grams per million Btu. However, a comparison of Figures 4 and 5 with Figure 1 shows that our model is superior to sodium oxide as a predictor of fouling deposit weight.

The error associated with any individual prediction is approximately 20-30 percent of the calculated fouling deposit weight. This figure is based on the range of differences between actual and predicted values for all the observations in both the development and test data sets. We found that 90 percent of the differences were <57 grams per million Btu, 75 percent of the differences were <28 grams per million Btu, and 50 percent of the differences were less than 15 grams per million Btu. Also, the largest errors occurred in samples that had very high actual fouling deposit weights. Large errors in this range are acceptable because, once deposit weights exceed 150 grams per million, a severe fouling problem exists and actual deposit weights are relatively unimportant. Accuracy is required, however, in the lower range of values, below 150 grams per million Btu. Our data indicate that equation 1 can be used to estimate fouling deposit weight to within 15-30 grams per million Btu, or less, an acceptable margin of error.

DISCUSSION

We believe that that fouling behavior of low-rank coal is predictable but that predictions will not be reliable when based on information from only one or two quality variables. Fouling is a complex phenomenon that involves a complex process (combustion) acting on a complex material (the coal). Therefore, predicting the fouling behavior of any coal will depend on a variety of coal components, their relative amounts, their mode of occurrence, and on furnace conditions.

A variety of components in the coal interact with one another during combustion to form or retard the formation of fouling deposits. These components include the total ash yield of the coal; sulfur content; and the amount of sodium, calcium, magnesium, potassium, and perhaps silica. The ash content, particularly the more siliceous minerals, forms the bulk or aggregate of the fouling deposits. Calcium, sulfur, sodium, etc., interact to influence how much and what types of materials will bind this siliceous/ash aggregate together and to the boiler tubes. Coal that has a low ash yield exhibits low fouling behavior. Coal that has a high ash yield exhibits extreme fouling behavior but only if there is sufficient adhesive material to amalgamate the deposit. Consequently, diluting high-sodium coal with ash material (roof rock for instance) may be inadvisable if ash yields are already very low. The aggregate or bulk phase of the fouling deposit is accounted for in our model by ash, by ash as part of the alkali ratio, and also by the TiO_2 factor, which we believe is indicative of the detrital component of the coal ash.

The binding, or hardening, of the deposits is, in our opinion, the least understood and probably the most complex aspect of the fouling deposit formation. In our view of fouling deposit formation, the sodium and potassium ions released by coal combustion compete with the calcium and magnesium ions for sulfur. There is evidence that potassium and sodium sulfates are present in fouling deposits or play a role in their formation (7). The picture is less clear for calcium and magnesium sulfates. However, in our opinion the calcium and magnesium sulfates do not participate as a binding phase in fouling deposit formation, but may, however, be incorporated into the deposit as inert material.

The sulfur, Ca/S, and alkali ratio factors in equation 1 all relate to this binding phase of the fouling deposit. The sulfur content is obviously important, for, without sulfur, no binding phase could be present. The calcium-sulfur ratio is a measure of how much sulfur will be bound by calcium and is, thus, not available to binding by sodium. The alkali ratio is a measure of the quantity of alkali elements that have been positively linked to deposit formation (sodium and potassium [8, 9]) relative to the elements that may have a negative impact on deposit formation (calcium and magnesium).

Finally, we stress that the model proposed in equation 1 is based principally on the degree of fit between the modeled data and the actual data, moderated by our perception of how various components in coal may behave during the formation of fouling deposits. The model is redundant because ash yield is represented in two places and the binding phase of the fouling deposits is represented by three terms. Two factors cause this redundancy. First, the mode of occurrence of the elements in the model affects the reactivity of the elements, in fouling deposit formation. Our model does not take mode of occurrence into account. Second, the development and test data sets are heavily biased towards moderate fouling coals. Only a few examples of coal that had extreme fouling behavior were available for inclusion in the data set. Inclusion of more low and high fouling coal samples in the data set might clarify the situation and result in a less redundant and more theoretically sound model. However, given the data currently available, this model does a good job of accurately predicting fouling behavior and it is clearly an improvement over the conventional (sodium) index currently in use.

CONCLUSIONS

1. We have developed a new model for predicting the fouling behavior of low rank coal. The model is based on commonly available coal quality data.
2. The proposed model has the potential to provide accurate quantitative estimates of fouling deposit weight per million Btu.
3. This model is more accurate in predicting fouling behavior than the sodium index.
4. Actual combustion tests of unknown coals need to be conducted to fully test the utility of this model.
5. The fouling potential of a coal cannot be adequately evaluated by using one or two compositional variables. A multivariate approach is more apt to yield reliable evaluations of fouling behavior.

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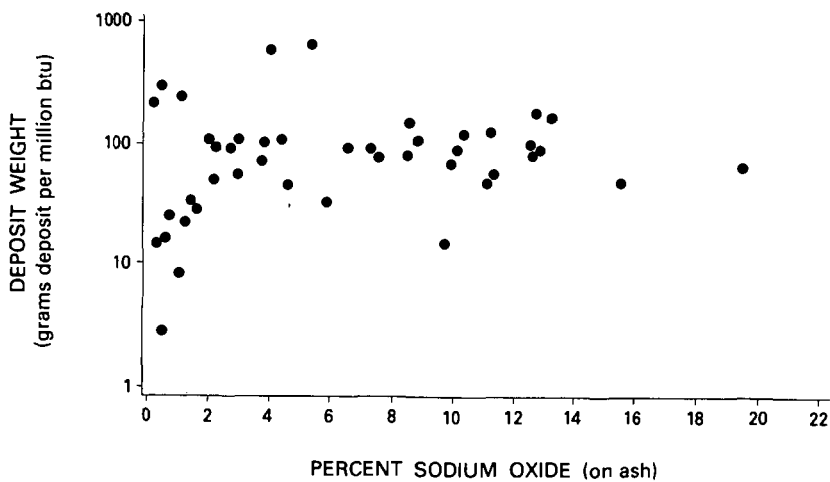


Figure 1.--Relation of sodium content to Fouling Deposit Weight.

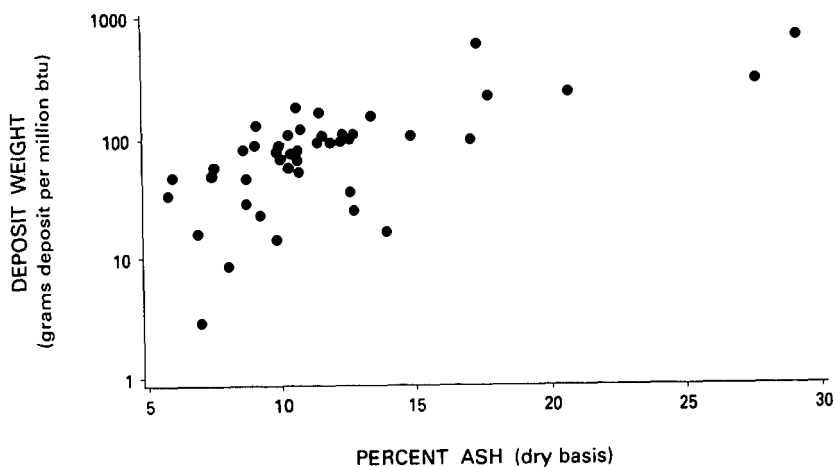


Figure 2.--Relation of coal ash yield to Fouling Deposit Weight.

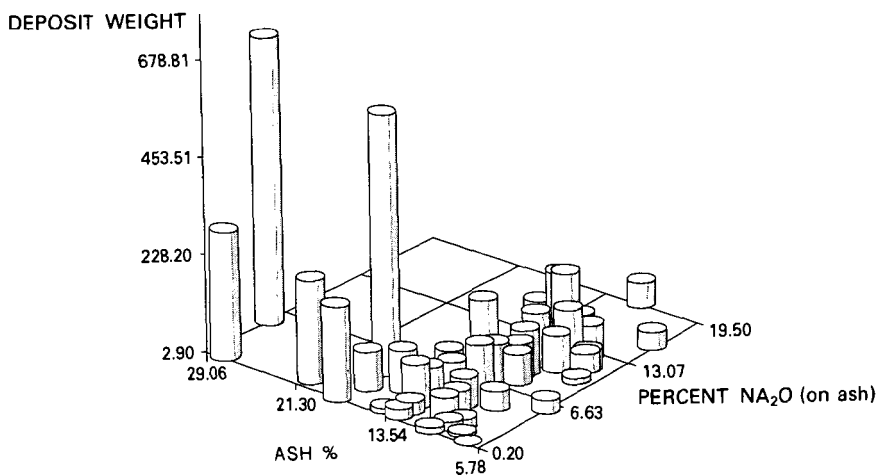


Figure 3.--Relation of ash and sodium contents to Fouling Deposit Weight.

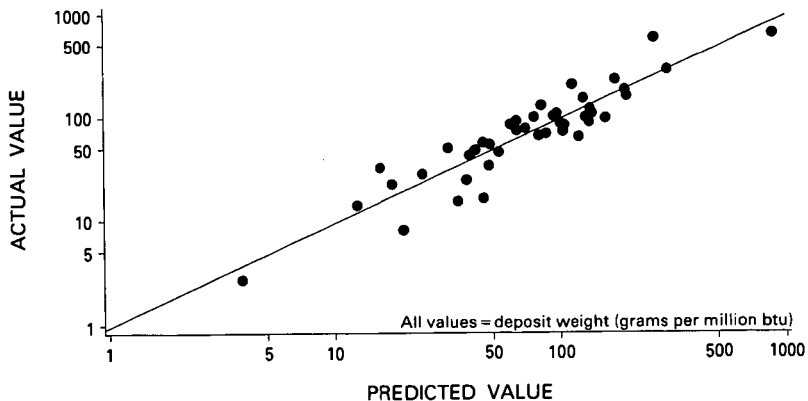


Figure 4.--Log/log plot of actual versus predicted Fouling Deposit Weight using our multivariate model (development data).

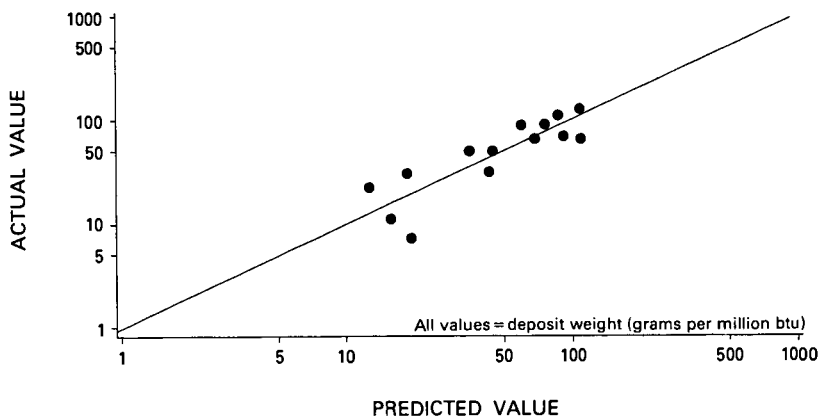


Figure 5.--Log/log plot of actual versus predicted Fouling Deposit Weight using our multivariate model (test data).

Table 1.--List of variables included in multivariate statistical analysis

| Variable | Mean | Range | Transform* Function |
|---|-------|---------------|------------------------|
| Ash (dry) | 11.73 | 5.78 - 29.06 | Log(10) |
| Btu (dry) | 10634 | 8400 - 12110 | - |
| Carbon (daf=dry ash-free) | 71.89 | 68.81 - 77.94 | - |
| Hydrogen (daf) | 4.75 | 2.78 - 5.73 | Square |
| Nitrogen (daf) | 1.16 | 0.99 - 1.86 | - |
| Oxygen (daf) | 20.68 | 15.73 - 24.49 | - |
| Volatile Matter (daf) | 48.25 | 42.41 - 55.13 | - |
| Sulfur (dry) | 1.29 | 0.29 - 4.13 | Log(10) |
| SiO ₂ (sulfate-free ash) | 32.75 | 15.20 - 61.50 | - |
| Al ₂ O ₃ (sulfate-free ash) | 15.02 | 8.50 - 22.90 | - |
| TiO ₂ (sulfate-free ash) | 0.68 | 0.20 - 1.70 | Log(10) |
| Fe ₂ O ₃ (sulfate-free ash) | 11.62 | 1.80 - 24.50 | - |
| CaO (sulfate-free ash) | 25.45 | 6.00 - 45.70 | - |
| MgO (sulfate-free ash) | 7.06 | 0 - 13.00 | - |
| K ₂ O (sulfate-free ash) | 0.61 | .10 - 2.50 | Log(10) |
| Na ₂ O (sulfate-free ash) | 6.26 | .20 - 19.5 | Sq. Root |
| Silicon (dry coal) | 1.64 | .43 - 7.71 | Log(10) |
| Aluminum (dry coal) | 0.78 | .27 - 2.78 | Log(10) |
| Sodium (dry coal) | 0.39 | .02 - 1.34 | Sq. Root |
| Calcium (dry coal) | 1.59 | .27 - 2.70 | - |
| SiO ₂ /Al ₂ O ₃ | 2.25 | 1.11 - 5.02 | Log(10) |
| Ca/S (dry coal) | 1.83 | .27 - 9.26 | Log(10) |
| Base-Acid Ratio | 1.21 | .22 - 3.15 | - |
| Alkali Ratio | 2.75 | .14 - 23.48 | Log(10) |
| Deposit Weight (gm/10 ⁶ Btu) | 112.7 | 2.90 - 678.81 | Log(10) |

*Function applied to those variables whose natural frequency distribution did not approximate a normal distribution. Transformed values do approximate a normal distribution.

All values except deposit weight, Btu, and ratios are percentages on basis shown.

Table 2.--Coal quality variables that significantly correlate with fouling deposit weight (g/million Btu)

| Variable | Correlation Coefficient |
|---|-------------------------|
| Ash (percent wt. of dry coal) | 0.67 |
| Sulfur (percent wt. of dry coal) | 0.49 |
| Btu/lb (dry coal) | -0.61 |
| TiO ₂ (percent wt. of sulfate-free ash) | 0.39 |
| K ₂ O (percent wt. of sulfate-free ash) | 0.36 |
| Volatile Matter (daf) | 0.52 |
| Si (percent wt. of dry coal) | 0.43 |
| Na (percent wt. of dry coal) | 0.49 |
| Al (percent wt. of dry coal) | 0.44 |
| Alkali Ratio | 0.65 |
| Na ₂ O (percent wt. of sulfate-free ash) | NS* |

*NS = not significant

Table 3.--List of coal quality variables used in prediction of fouling deposit weight (g/million Btu)

| Quality Parameter | Basis |
|------------------------------------|---------------------------------|
| Titanium Oxide (TiO ₂) | percent wt. of sulfate-free ash |
| Ash Yield | percent wt. of dry coal |
| Total Sulfur | percent wt. of dry coal |
| Calcium Oxide (CaO) | percent wt. of sulfate-free ash |
| Sodium Oxide (Na ₂ O) | percent wt. of sulfate-free ash |
| Potassium Oxide (K ₂ O) | percent wt. of sulfate-free ash |
| Magnesium Oxide (MgO) | percent wt. of sulfate-free ash |